THEORY AND MODELING OF NANOSCARBON PHASE STABILITY

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Keywords: nanodiamond, bucky-diamond, theory, simulation, phase stability.

Abstract

The transformation of nanodiamonds into carbon-onions (and vice versa) has been observed experimentally and has been modelled computationally at various levels of sophistication [1,2]. Also, several analytical theories have been derived (by a number of research groups) to describe the size, temperature and pressure dependence of this phase transition [1]. However, in most cases a pure carbon-onion or nanodiamond is not the final product. More often than not an intermediary is formed, known as a bucky-diamond, with a diamond-like core encased in an onion-like shell. This has prompted a number of studies investigating the relative stability of nanodiamonds, bucky-diamonds, carbon-onions and fullerenes, in various size regimes. Presented will be a review outlining results of numerous computational and theoretical studies examining the phase stability of carbon nanoparticles, to clarify the complicated relationship between fullerenic and diamond structures at the nanoscale [1].

REFERENCES

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